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# *EXCITATION OF THE 2s AND 2p LEVELS OF THE HYDROGEN ATOM BY SLOW ELECTRONS*

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The cross sections for excitation of the 2s and 2p levels of the hydrogen atom by slow electrons are calculated by taking into account exchange and all coupling between the 1s, 2s, and 2p levels. The system of four (for $L = 0$, three) integro-differential equations was solved by a non-iteration method for a total orbital momentum $L < 2$ and by an iteration method for $L = 3$ and 4. The calculated $\sigma$(1s—2s) value practically agrees with that from Lichten and Schultz's experiment; at low energies $\sigma$(1s—2p) considerably exceeds the experimental value obtained by Fite et al.

RECENTLY much attention has been paid to collisions between slow electrons and hydrogen atoms. The Born approximation turns out to be insufficiently accurate at low energies. The method of distorted waves without account of strong coupling and exchange leads to highly over valued cross sections [1]. Marriott [2] and Smith [3] calculated the excitation cross sections of the 2s level with account of exchange and the strong coupling of the levels 1s—2s [2,3] and 1s—2s—3s [3]. The results have demonstrated that exchange plays a major role and coupling with the 3s level a less considerable role. Comparison of Marriott's result [2] with an earlier variational calculation [4] has created the impression that the 1s—2s coupling plays a major role. However, a direct numerical integration [5] has shown that the variational calculation is not accurate and that this coupling influences little the 1s—2s cross section.

A large influence can be expected from the mutual coupling of the 2s and 2p levels. The importance of this coupling was demonstrated in the Born approximation [6] and by numerical solution of the system of differential equations without account of exchange [7,8].

In the present work the cross sections were calculated with complete account of the exchange and all the couplings between the 1s—2s—2p levels. The problem was solved in the total orbital momentum and projection representation [9]. The calculations were made for five momenta: $0 \leq L \leq 4$. Both scattered waves (with momenta $L \pm 1$) were taken into consideration in the excitation of the 2p level for $L > 0$. The system of four (three in the case $L = 0$) coupled integro-differential equations for $L \leq 2$ was solved by the non-iterational method used by Marriott [2].[1)] An iteration calculation was used for $L = 3$ and 4.

Table I lists the partial averaged cross sections $\sigma_L$ and average, direct, and exchange cross sections summed over $L = 0, 1, \ldots, 4$.

The amplitudes of the direct and exchange transitions are

$$f_L = \tfrac{1}{2}(f_L^+ + f_L^-), \quad g_L = \tfrac{1}{2}(f_L^+ - f_L^-), \tag{1}$$

where $f_L^+$ and $f_L^-$ are the singlet and triplet amplitudes. The singlet, triplet, and averaged cross sections have the form

$$\sigma_L^{\pm} = |f_L|^2 + |g_L|^2 \pm 2\mathrm{Re}(f_L g_L^*), \tag{2}$$

$$\sigma_L = |f_L|^2 + |g_L|^2 - \mathrm{Re}(f_L g_L^*). \tag{3}$$

Table I lists also the elastic-scattering cross sections. At an electron momentum $k = 0.9$ a.u. the agreement between calculation and experiment [11] is satisfactory. There are no experimental data for $k \geq 1$. Comparison with earlier calculations [12,3] shows that an account of the strong coupling influences the total elastic cross section relatively little. An account of the exchange greatly increases the elastic cross section, owing to the addition of the exchange and interference terms, but the direct scattering section changes little in this case as compared with the calculation without the exchange [13,7].

The situation is reversed upon excitation: the interference term almost completely cancels out

[1)]An analogous non-iterational method which reduces to the solution of a system of Volterra differential equations and a system of algebraic equations was previously proposed by Drukarev.[10]

Table I

| | k, a. u. | Partial sections in $\pi a_0^2$ units | | | | | Sum over $L = 0; 1, \ldots; 4$ in $\pi a_0^2$ units | | |
|---|---|---|---|---|---|---|---|---|---|
| | | $\sigma_0$ | $\sigma_1$ | $\sigma_2$ | $\sigma_3$ | $\sigma_4$ | $\sigma$ | $\lvert f\rvert^2$ | $\lvert g\rvert^2$ |
| 1s — 1s | 0.9 | 4.136 | 1.737 | 0.132 | 0.024 | 0.007 | 6.035 | 3.485 | 1.221 |
| | 1.0 | 3.172 | 1.382 | 0.159 | 0.025 | 0.008 | 4.746 | 2.723 | 0.908 |
| | 1.2 | 1.956 | 0.897 | 0.130 | 0.026 | 0.010 | 3.019 | 1.629 | 0.632 |
| | 1.5 | 1.053 | 0.522 | 0.092 | 0.019 | 0.009 | 1.695 | 0.967 | 0.294 |
| | 2.0 | 0.466 | 0.266 | 0.076 | 0.023 | 0.009 | 0.839 | 0.588 | 0.073 |
| 1s — 2s | 0.9 | 0.055 | 0.075 | 0.062 | 0.018 | 0 | 0.210 | 0.138 | 0.160 |
| | 1.0 | 0.080 | 0.139 | 0.103 | 0.031 | 0.009 | 0.362 | 0.268 | 0.221 |
| | 1.2 | 0.043 | 0.099 | 0.061 | 0.028 | 0.018 | 0.250 | 0.214 | 0.114 |
| | 1.5 | 0.017 | 0.065 | 0.032 | 0.011 | 0.010 | 0.135 | 0.135 | 0.028 |
| | 2.0 | 0.008 | 0.031 | 0.025 | 0.012 | 0.006 | 0.081 | 0.089 | 0.006 |
| 1s — 2p | 0.9 | — | 0.094 | 0.102 | 0.051 | 0.001 | 0.249 | 0.250 | 0.124 |
| | 1.0 | — | 0.113 | 0.248 | 0.197 | 0.053 | 0.612 | 0.617 | 0.251 |
| L — 1 | 1.2 | — | 0.061 | 0.297 | 0.290 | 0.189 | 0.837 | 0.950 | 0.246 |
| | 1.5 | — | 0.013 | 0.121 | 0.199 | 0.198 | 0.533 | 0.634 | 0.070 |
| | 2.0 | — | 0.002 | 0.030 | 0.068 | 0.093 | 0.193 | 0.226 | 0.010 |
| 1s — 2p | 0.9 | 0.038 | 0.047 | 0.015 | 0.002 | 0 | 0.102 | 0.062 | 0.097 |
| | 1.0 | 0.039 | 0.075 | 0.051 | 0.006 | 0.001 | 0.171 | 0.096 | 0.151 |
| L + 1 | 1.2 | 0.044 | 0.060 | 0.046 | 0.010 | 0.003 | 0.163 | 0.124 | 0.122 |
| | 1.5 | 0.028 | 0.017 | 0.008 | 0.007 | 0.006 | 0.066 | 0.068 | 0.022 |
| | 2.0 | 0.009 | 0.004 | 0.001 | 0.002 | 0.004 | 0.019 | 0.021 | 0.003 |

the contribution of the exchange excitation. In some cases the average cross section is even smaller than the direct excitation cross section. The exchange cross section decreases rapidly with increasing energy or momentum.

The cross section $\sigma$(1s—2s) was measured in many experiments [14,15]; Lichten and Schultz [14] measured also the quantity $\frac{1}{2}|g|^2$. Their data exceed those given by Stebbings, Fite, et al [15] by a factor of more than three, but the experimental curves have the same shape. It turned out later [16] that the results of Stebbings, Fite et al [15] should be increased by 1.5 times. This still left a disparity by a factor 2.25. The absolute cross section in [14] was determined highly inaccurately (with an error $\pm 0.14\pi a_0^2$, where $a_0$ is the Bohr radius), and was chosen relatively arbitrarily in that the comparison with the Born cross section was made at 40 eV. In addition, the data of [14] are made somewhat ambiguous by the lack of exact information on the cross section $\sigma$(1s—3p).

Starting from an estimate of the role of the 2s—2p coupling in the second Born approximation, Hummer and Seaton [17] advanced the hypothesis that calculations with account of the exchange in the 2s—2p coupling will lead to agreement with the corrected data of Fite et al [16]. Our results, however, show that this is not the case.

In Figs. 1 and 2 the results are compared with experiment and with other calculations. For the total cross section, the missing part $\sum_{L=5}^{\infty} \sigma_L$ was taken from the work of Burke and Seaton [6], where an approximate calculation of the strong coupling was made within the framework of the first Born approximation. Our results both for the total averaged cross section $\sigma$(1s—2s) and for the exchange cross section are in practical agreement

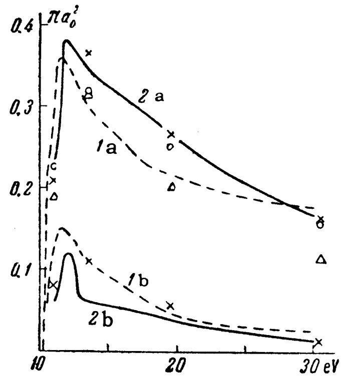


FIG. 1. Cross sections for the excitation of the 2s level (in units of $\pi a_0^2$): a – average cross section: b – (1/2)$|g|^2$. Curves 1a, b – experiment,[14] x – present calculation. In curves 2a, b $Q_2$ is the sum of partial cross sections over L = 0, 1, 2, calculated by the method of distorted waves with account of exchange (MDWE);[4] o – $Q_2$ with account of 1s–2s coupling;[3] Δ – $Q_2$ from present calculation.

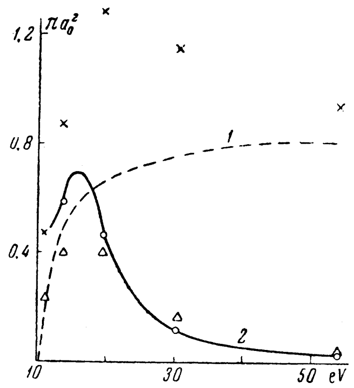


FIG. 2. Excitation cross sections of the 2p level (in units of $\pi a_0^2$). Curve 1 – $\sigma_\perp$ (experiment)[18], x – $\sigma_\perp$ (present calculation); curve 2 – $Q_2$, MDWE, numerical integration,[5] o – $Q_2$, MDWE, variational calculation,[20] Δ – $Q_2$, present calculation. In $Q_2$ with L = 1 and 2 the contribution of the wave departing with momentum L + 1 is disregarded.

with the experiment[14]. It is little likely that an account of the coupling with 3s, 3p and other levels can change the cross section appreciably (particularly when $k \geq 1.2$). It is therefore desirable to know more accurately the experimental value of the absolute cross section. It would also be necessary to make the value of $\sigma$(1s—3p) more precise.

The quantity measured in the experiments[18] for the 2p level was not $\sigma_{\perp}$(1s—2p) but $\sigma$(1s—2p), obtained by counting the photons emitted perpendicular to the electron beam, followed by calculation of the total cross section under the assumption that the photon distribution is isotropic.

According to the theory of Percival and Seaton [19] we have

$$\sigma_{\perp}(1s-2p) = 0.918\,\sigma(1s-2p) + 0.246\,\sigma(1s-2p, 0), \quad (4)$$

and the radiation polarization, in per cent, is

$$P(2p) = \frac{\sigma(1s-2p,0) - \sigma(1s-2p, \pm 1)}{2.375\,\sigma(1s-2p, 0) + 3{,}749\,\sigma(1s-2p, \pm 1)} \cdot 100, \quad (5)$$

where $\sigma$(1s—2p, 0) and $\sigma$(1s—2p, ±1) are the excitation cross sections of the 2p level with projections of the momentum of the atomic electron on the direction of the incident electron respectively equal to 0 or ±1.

Table II lists the values of $\sigma$(1s—2p, ±1), $\sigma$(1s—2p, 0) and P(2p) (the cross sections are in units of $\pi a_0^2$).

**Table II**

| k, a. u. | $\sigma$ (1s—2p, ±1) | $\sigma$ (1s—2p, 0) | P (2p), % |
|---|---|---|---|
| 0.9 | 0.068 | 0.215 | 19.2 |
| 1.0 | 0.096 | 0.602 | 28.3 |
| 1.2 | 0.128 | 0.897 | 29.5 |
| 1.5 | 0.197 | 0.673 | 20.4 |
| 2.0 | 0.237 | 0.433 | 10.2 |

When k = 2 atomic units (energy 54 eV) the theoretical cross section $\sigma_{\perp}$(1s—2p) is close to the experimental one, and the polarization is within the experimental errors. At lower energies, the theoretical cross section is larger and the polarization much smaller than the experimental value.

The calculated total cross section $\sigma$(1s—2p) differs little from the results of Khashaba and Massey[20]. Account of strong coupling greatly reduces the sum of the first three partial cross sections at energy < 20 eV. But in this case $\sigma_3$ and $\sigma_4$ increase in comparison with the Born-Oppenheimer and the Born approximations. For the cross section $\sigma_1$ and $\sigma_2$, the role of the wave outgoing with momentum L+1 also increases appreciably.

With increasing energy and momentum the partial cross sections approach the Born cross section[6]. This was also confirmed by calculations carried without account of exchange for L = 5 and 6. We note that when L = 4 the value of $\sigma_L$ differs little from those calculated without account of exchange[8].

A more detailed exposition of the results, containing the elements of the T matrix and the cross sections of the transitions from the excited states will be published in the Trudy of the Physics Institute of the Latvian Academy of Sciences.

Note added in proof (October 15, 1962). Dr. Seaton graciously communicated to us the results of a similar calculation by Burke, Shea, and Smith (submitted to Physical Review), which is in agreement with ours. An essential difference is observed only in the values of the radiation polarization.

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